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SOLUTION OF EVAPORATION AND CONDENSATION PROBLEMS BASED ON THE CONJUGATE APPROACH

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KEY WORDS

Heat and mass transfer through an interface, evaporation and condensation, Boltzmann kinetic equation, velocities distribution function of molecules, intermolecular interaction potential.

ABSTRACT

At evaporation and condensation transport of mass and energy is realized as in vapor and in condensed phase. Generally liquid and vapor phases should be considered as a single combined system at each time step when non-steady problem is solved. Solution of this problem is enough difficult because the typical time of heat transfer processes in liquid domain is very different than the typical time of such processes in vapor.

In this paper the processes in vapor phase near vapor-liquid interface are described on the base of the Boltzmann kinetic equation (BKE). It is should be noted that the boundary conditions on the liquid-vapor interface must be prescribed for this equation solution. One approach for deriving these boundary conditions is to apply methods of molecular dynamics (MD) simulation. For BKE solution detailed information about particles velocities and coordinates are not required. Only the velocities distribution function of vapor molecules flying from the liquid-vapor interface is needed. Direct inclusion of molecular dynamics modeling in the algorithm of the Boltzmann equation solution would lead to unreasonably high computational time and memory costs. The main objectives of this study are to develop a method of transport problems solving in a two-phase (condensate–vapor) system that accounts the peculiarities of the atom–interface interactions and to obtain the distribution function for the evaporated atoms.

Distribution function of vapor molecules flying from condensate is determined strongly by binding energy which evaporated atom or molecule should overcome for transition from liquid to vapor. This energy value depends on atom position, nearest neighbors [1] and intensity of thermal motion i.e. liquid temperature [2]. Thus potential energy for a set of local neighbouring particles is used. Simulation taking into account these peculiarities gives results which can be approximated by the following formula for determination of binding energy value ε_s as liquid temperature T function:

$$\varepsilon_s = kT \frac{\varepsilon_{s0}}{\varepsilon} Cos\left(\frac{\pi T}{2T_k}\right), \tag{1}$$

where k is the Boltzmann constant, ε_{s0} is minimal potential energy for the set of neighboring motionless particles, ε is Lennard-Jones molecule-pair potential parameter (potential well), T_k is an extreme temperature above which the energy of the particle interactions is negligible compared with the kinetic energy of the thermal movement. T_k is assumed to be close to the critical-point temperature.

Figure 1 illustrates the scheme of distribution function determination. In this figure f is the distribution function of condensate atoms (left picture), f^r is the distribution function of vapor atoms (right picture), ξ and ξ^r are the velocities of liquid and vapor atoms correspondingly, $\xi_x^r = \sqrt{\xi_x^2 - u_s^2}$, $u_s = \sqrt{2|\varepsilon_s|/m}$, m is

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the mass of atom, x is the Cartesian coordinate normal to interface surface. Vapor distribution function is determined from equality of mass flux densities in liquid and vapor. Details see in paper [2].
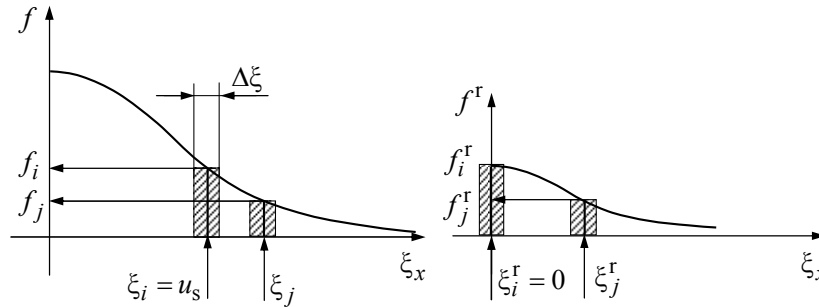
Figure 1: Distribution function determination.

The proposed approach gives the possibilities to obtain the equilibrium saturation vapor–liquid lines [3] as well as to solve different non-steady evaporation–condensation problems.

Above mentioned method was applied to an evaporation–condensation problem. Here, left and right boundaries represent interfaces on which evaporation and condensation occur. The initial vapor density in the studied region was set close to zero. The temperatures of boundary surfaces were set as follows: $T_1 = 130$ K on the left and $T_2 = 110$ K on the right. Dependences of vapor density on coordinate x in the non steady evaporation–condensation problem at fig. 2 are presented. Fig. 3 depicts the according steady solution. $T_0 = 110$ K and density of saturated vapor for argon $\rho_0 = 33.49$ kg/m^3 at T_0, $\lambda = 3.08 \cdot 10^{-9}$ m is the length of free path at T_0 and ρ_0. In the fig. 2 curves are given with a time step $1 \cdot 10^{-9}$ s.
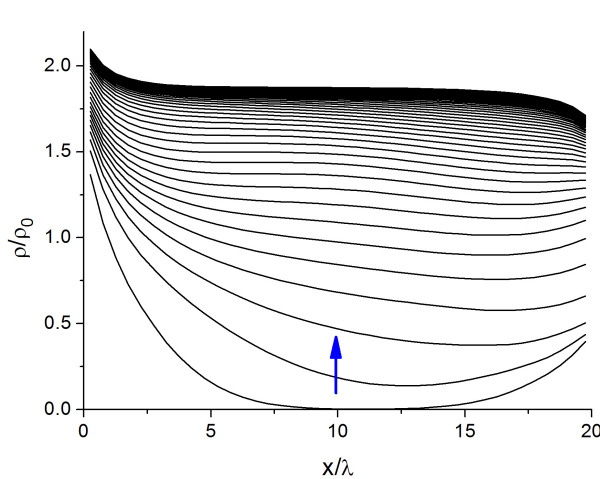
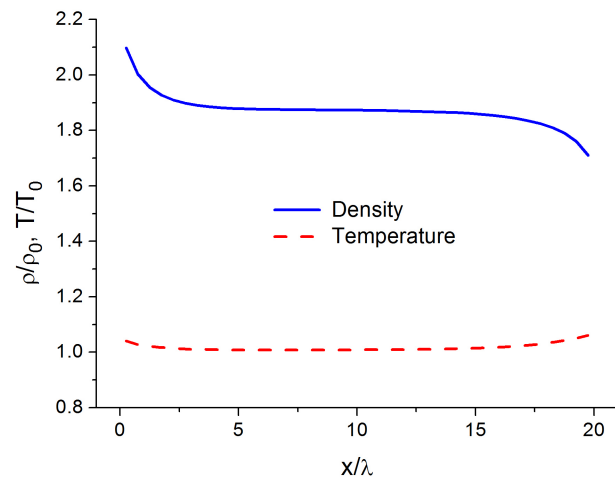**Figure 2:** Dependence of vapor density on coordinate x at different time moments.

Figure 3: Dependence of vapor density and temperature on coordinate x: steady solution.

Acknowledgements

References

[1] Anisimov, S.I. and V. V. Zakhovskii, V.V. (1993). Evaporation of a liquid. *JETP Lett.*, 57, No.2, 99–102.
[2] Shishkova, I.N. and Kryukov, A.P. (2016). Approximate solution of a conjugate problem of heat and mass transfer through an interface. *Journal of Engineering Physics and Thermophysics*, 89, 499–505.
[3] Shishkova, I.N., Kryukov, A.P. and Levashov, V.Yu. (2017). Study of evaporation–condensation problems: From liquid through interface surface to vapor. *Int. J. of Heat and Mass Transfer*, 112, 926–932.